

Defect engineered Ti-MOFs and their applications

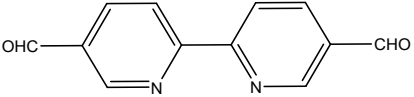
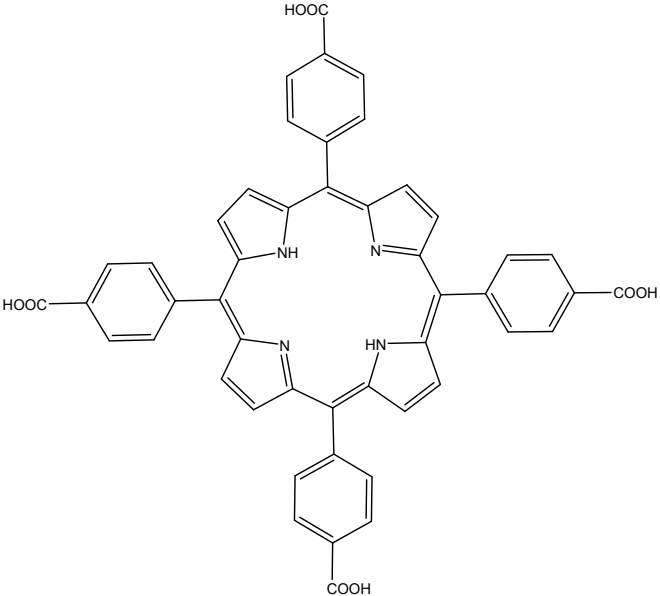
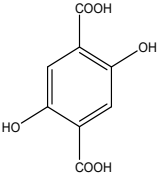
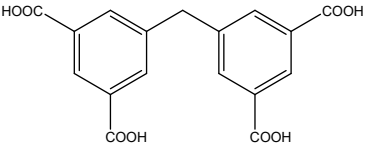
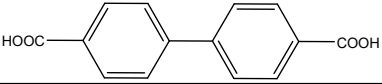
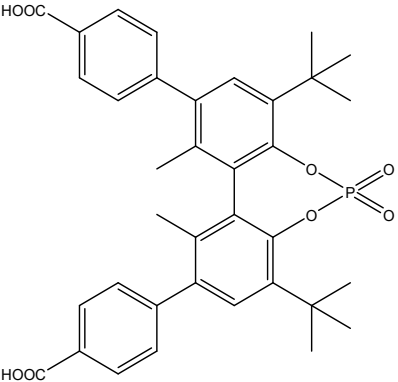
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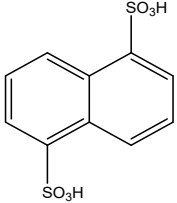
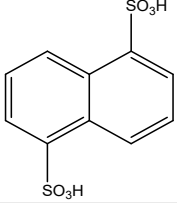
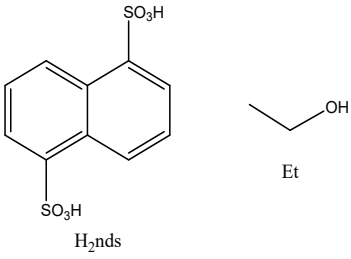
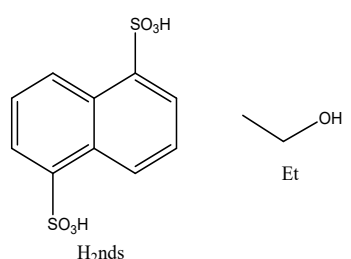
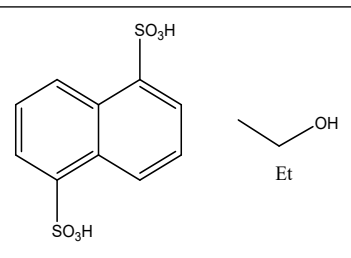
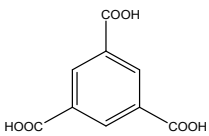
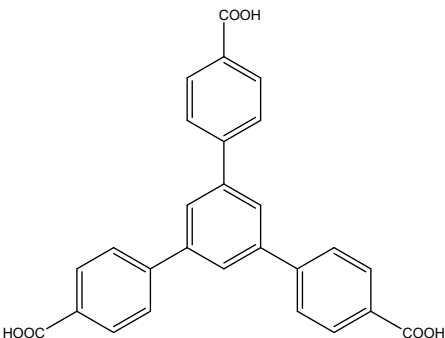
Tab. S1 Summary of linker structural formulas for Ti MOFs.

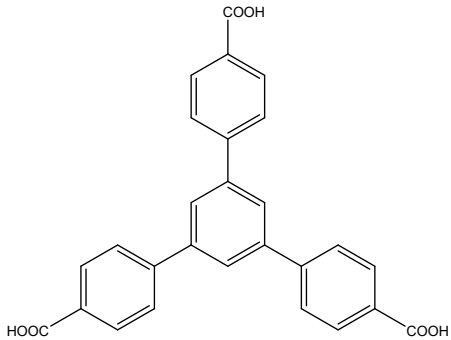
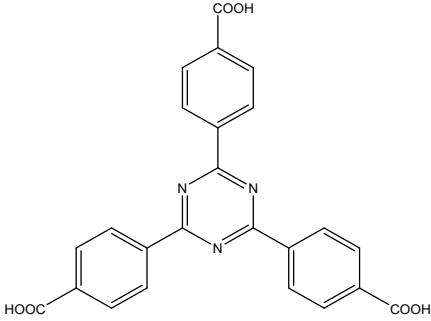
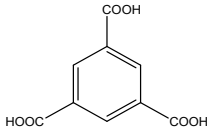
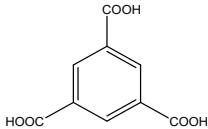
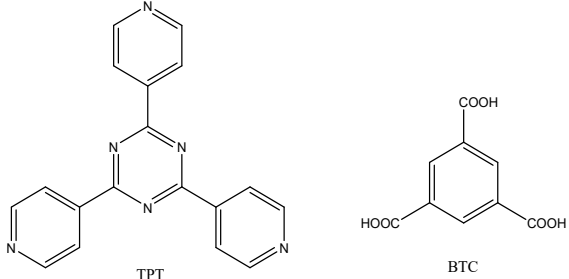
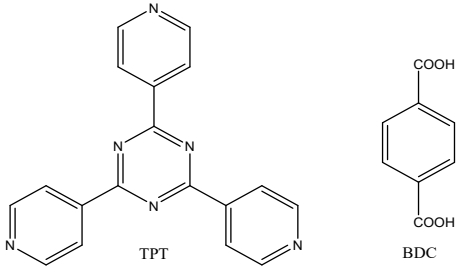
Entry	Material	Linker	Structure
1	MIL-22	H ₂ O ₃ P-(CH ₂)-PO ₃ H ₂	
2	MIL-25 ₂	H ₂ O ₃ P-(CH ₂) ₂ -PO ₃ H ₂	
3	MIL-25 ₃	H ₂ O ₃ P-(CH ₂) ₃ -PO ₃ H ₂	
4	FIR-136	H ₂ nds , 1,4-butanediol	
5	FIR-137	H ₂ nds , 1,5-pentanediol	
6	NTU-9	DOBDC	
7	MIL-167	DOBDC	

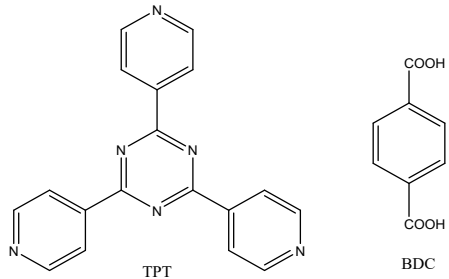
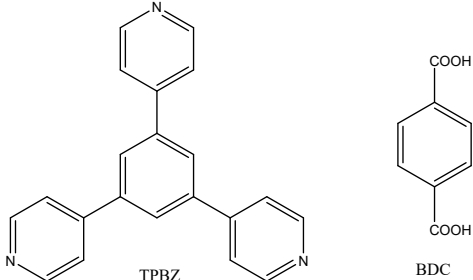
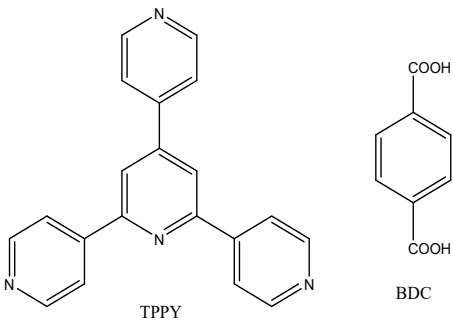
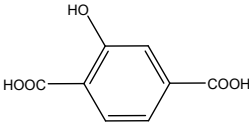

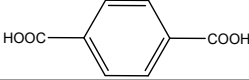
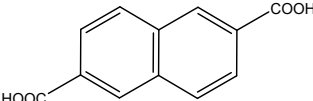
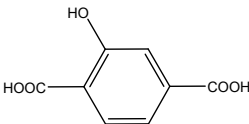
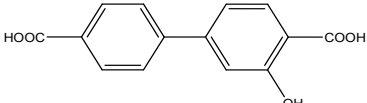
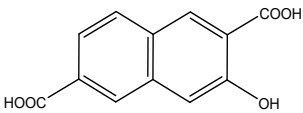
8	MIL-168	DOBDC	<p>Chemical structure of 2,4,6-trihydroxy-1,3,5-tricarboxylate (DOBDC), a benzene ring with hydroxyl groups at positions 2, 4, and 6, and carboxylic acid groups at positions 1, 3, and 5.</p>
9	FIR-117	DOBDC	<p>Chemical structure of 2,4,6-trihydroxy-1,3,5-tricarboxylate (DOBDC), a benzene ring with hydroxyl groups at positions 2, 4, and 6, and carboxylic acid groups at positions 1, 3, and 5.</p>
10	FIR-118	DOBDC	<p>Chemical structure of 2,4,6-trihydroxy-1,3,5-tricarboxylate (DOBDC), a benzene ring with hydroxyl groups at positions 2, 4, and 6, and carboxylic acid groups at positions 1, 3, and 5.</p>
11	FIR-119	DOBDC	<p>Chemical structure of 2,4,6-trihydroxy-1,3,5-tricarboxylate (DOBDC), a benzene ring with hydroxyl groups at positions 2, 4, and 6, and carboxylic acid groups at positions 1, 3, and 5.</p>
12	FIR-120	DOBDC	<p>Chemical structure of 2,4,6-trihydroxy-1,3,5-tricarboxylate (DOBDC), a benzene ring with hydroxyl groups at positions 2, 4, and 6, and carboxylic acid groups at positions 1, 3, and 5.</p>
13	MUV-11	H ₄ bdha	<p>Chemical structure of 1,3-bis(hydroxyamino)benzene-5,7-dicarboxylic acid (H₄bdha), a benzene ring with hydroxylamino groups at positions 1 and 3, and carboxylic acid groups at positions 5 and 7.</p>
14	Ti-CAT-5	H ₆ THO	<p>Chemical structure of 1,3,5-tris(2,4,6-trihydroxyphenyl)benzene (H₆THO), a central benzene ring with three 2,4,6-trihydroxyphenyl groups attached at positions 1, 3, and 5.</p>
15	MOF-217	TDHT	<p>Chemical structure of 2,4,6-tris(3,5-dihydroxyphenyl)-1,3,5-triazine (TDHT), a central 1,3,5-triazine ring with three 3,5-dihydroxyphenyl groups attached at positions 2, 4, and 6.</p>


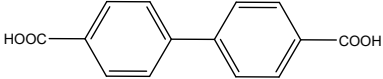
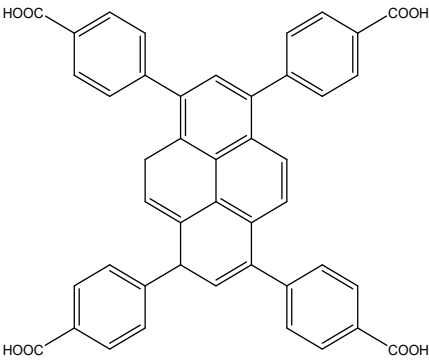
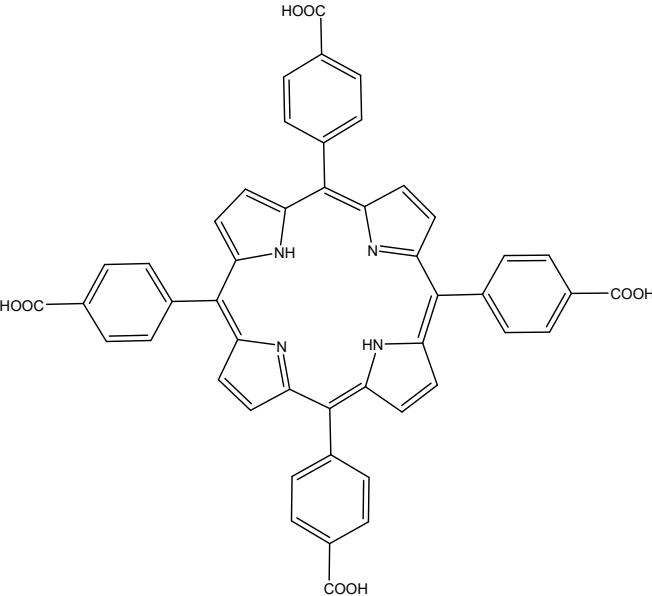
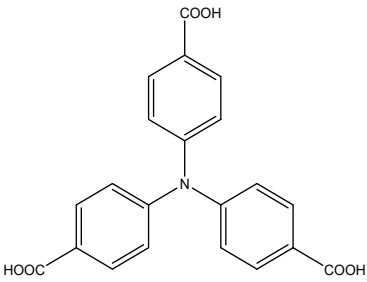
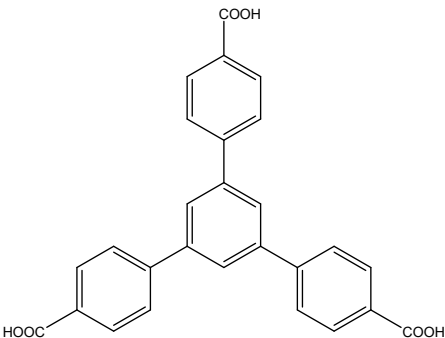
16	MIL-125	BDC	
17	FIR-125	H ₂ odb	
18	FIR-126	H ₂ sodb	
19	FIR-127	H ₂ nsa	
20	MIP-207	BTC	
21	COK-69	H ₂ CDC	
22	Ti-MIL-101	BDC	
23	Ti-MIL-100	BTC	
24	MTM-1	INA	
25	MOF-901	AB, BDA	 AB BDA
26	MOF-902	AB, BPDA	 AB BPDA

27	NU-2300	[2,2'-Bipyridine]-5,5'-dicarbaldehyde	 <p>The structure shows two pyridine rings connected at their 2-positions. Each ring has an aldehyde group (-CHO) at the 5-position.</p>
28	PCN-22	TCPP	 <p>The structure is a porphyrin-like macrocycle with four nitrogen atoms. Each nitrogen is coordinated to a central point. The four meso-positions of the macrocycle are substituted with para-carboxyphenyl groups (-C₆H₄-COOH).</p>
29	MIL-169	H ₄ DOBDC	 <p>The structure is a benzene ring with a carboxylic acid group (-COOH) at the 1-position, hydroxyl groups (-OH) at the 2 and 4 positions, and another carboxylic acid group (-COOH) at the 3-position.</p>
30	MIL-177-LT	H ₄ mdip	 <p>The structure consists of two benzene rings connected by a methylene (-CH₂-) bridge at their 1-positions. Each ring has carboxylic acid groups (-COOH) at the 2 and 4 positions.</p>
31	Ti ₃ -BPDC	H ₄ BPDC	 <p>The structure is a biphenyl system with two benzene rings connected at their 1-positions. Each ring has a carboxylic acid group (-COOH) at the 4-position.</p>
32	1-Ti	H ₃ L	 <p>The structure is a complex porphyrin-like macrocycle with four nitrogen atoms. It features a central phosphorus atom coordinated to two of the nitrogens. The macrocycle is substituted with tert-butyl groups and two para-carboxyphenyl groups (-C₆H₄-COOH).</p>

33	FIR-131	H ₂ nds	 <p>Chemical structure of 1,4-naphthoquinone-2,7-diol, a naphthalene ring system with two hydroxyl groups at the 2 and 7 positions.</p>
34	FIR-132	H ₂ nds	 <p>Chemical structure of 1,4-naphthoquinone-2,7-diol, a naphthalene ring system with two hydroxyl groups at the 2 and 7 positions.</p>
35	FIR-133	H ₂ nds, Et	 <p>Chemical structures of 1,4-naphthoquinone-2,7-diol and ethanol. The naphthalene structure is labeled with SO₃H groups at the 2 and 7 positions and H₂nds below it. The ethanol structure is labeled with Et below it.</p>
36	FIR-134	H ₂ nds, Et	 <p>Chemical structures of 1,4-naphthoquinone-2,7-diol and ethanol. The naphthalene structure is labeled with SO₃H groups at the 2 and 7 positions and H₂nds below it. The ethanol structure is labeled with Et below it.</p>
37	FIR-135	H ₂ nds, Et	 <p>Chemical structures of 1,4-naphthoquinone-2,7-diol and ethanol. The naphthalene structure is labeled with SO₃H groups at the 2 and 7 positions and H₂nds below it. The ethanol structure is labeled with Et below it.</p>
38	MUV-10	BTC	 <p>Chemical structure of 1,3,5-tricarboxybenzene, a benzene ring with three carboxylic acid groups at the 1, 3, and 5 positions.</p>
39	MUV-12	BTB	 <p>Chemical structure of 4,4'-(m-phenylene)-3,3'-bis(4-carboxyphenyl)benzoic acid, a central benzene ring with a carboxylic acid group at the 1 position and two 4-carboxyphenyl groups at the 3 and 3' positions, connected to a 4-carboxyphenyl group at the 4' position.</p>

40	LCU-402	BTB	
41	LCU-505	TATB	
42	MTV-MIL-100	BTC	
43	MUV-101	BTC	
44	ST-sod-Co,Ti	BTC, TPT	
45	CPM-223	BDC, TPT	

46	CPM-723	BDC, TPT	 <p>TPT</p> <p>BDC</p>
47	CPM-223-tpdz	BDC, TPBZ	 <p>TPBZ</p> <p>BDC</p>
48	CPM-223-tppy	BDC, TPPY	 <p>TPPY</p> <p>BDC</p>
49	CTOF-1	OBDC	
50	CTOF-2	BDC	
51	PCN-415	BDC	
52	PCN-416	NDC	
53	ZTOF-1	OBDC	
54		H ₃ OBPDC	
55	ZTOF-2	H ₃ ONDC	

56	MIL-91	N, N-PMP	
57	Ti-MFM-300	H ₄ BPDC	
58	ACM-1	H ₄ TBAPy	
59	DGIST-1	meso-TCPP	
60	ZSTU-1	H ₃ TCA	
61	ZSTU-2	BTB	

62	ZSTU-3	H ₃ BTCA	
63	MIL-177-HT	H ₄ mdip	
64	UCFMOF-4	QPDC	
65	UCFMOF-3	TPDC	
66	Ti-TBP	TBP/TCPP	
67	MIP-208	IPA	
68	COK-47	H ₂ BDA	
69	Ti-BPDC	H ₄ BPDC	

